



Proposal for building an ozone module for the soil-crop model STICS

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Proposal for building an ozone module for STICS

First, we present the way the impact of ozone (O₃) was already introduced into new or existing models (Kobayashi, 1997; AFRCWHEAT2-O₃ with Ewert and Porter, 2000; Van Oijen et al., 2004 and CERES-O₃ model with Lebard, 2005). Second, we discuss the way those approaches feed the conceptual framework of the new ozone module for the STICS model.

1. **Presentation of existing modelling approaches for O₃ effects on crop growth and development**

For every approaches, we detail the way (i) the O₃ influx into the plant, (ii) the O₃ inhibition of photosynthesis and (iii) the O₃ acceleration of leaf senescence, are calculated.

a. Kobayashi, 1997

i. O₃ inflow

The O₃ inflow is not actually calculated. The model consider a **daily damaging O₃ concentration** [O₃](d)¹ that is calculated as the excess of O₃ concentration beyond a background O₃ concentration under which there is no damage P₋[O_{3,b}]²:

$$[O_3](d) = [O_{3,a}](d) - P_{-}[O_{3,b}] \quad (1)$$

ii. O₃ effect on photosynthesis

The daily radiation use efficiency RUE(d) is reduced by a factor accounting for the daily damaging O₃ concentration [O₃](d) previously calculated (eq.1). This reducing factor also depends on the sensitivity of the crop to O₃, varying with the phenology, P_{pi}.

$$RUE_{O_3}(d) = (1 - P_{pi} \cdot [O_3](d)) \cdot RUE(d) \quad (2)$$

With P_{pi} = P_{pveg} during vegetative growth, and P_{pi} = P_{prep} during reproductive growth. P_{pveg} is assumed to be lower than P_{prep}, considering that the O₃ impact on photosynthesis is much greater during reproductive growth.

iii. O₃ effect on senescence

The natural senescence rate P_{α_r} is increased by a factor accounting for the daily damaging O₃ concentration [O₃](d) previously calculated (eq.1). This factor also depends on the sensitivity of the crop to O₃ during reproductive growth, P_{p_{rep}}. The daily LAI is thus calculated after having reached its maximum (LAI_{max}):

$$LAI(d) = LAI_{max} - P_{\alpha_r} \sum_{LAI_{max}day}^{Harvest\ day} (1 + P_{prep} \cdot [O_3](d)) \quad (3)$$

b. Ewert and Porter with AFRCWHEAT2-O₃, 2000

i. O₃ inflow

The **instantaneous O₃ uptake rate** O_{3,up} is calculated according to the stomatal conductance for O₃ which is the stomatal conductance for CO₂ g_{sc} corrected for the differences in the diffusivities of CO₂ and O₃ in the air with the ratio P_{f_DO₃} (Laisk et al., 1989):

$$O_{3,up} = [O_{3,a}] \cdot g_{sc} \cdot P_{f_{D}O_3} \quad (4)$$

¹ All parameters and variables are listed in annex 1

² All parameters, supposed to remain constant are preceded by "P₋"

ii. O₃ effect on photosynthesis

The short-term O₃ inhibition on photosynthesis is simulated through an O₃ dose effect factor $f_{O3,s}(d)$ (see eq.5 below) taking into account that:

- the short-term photosynthesis inhibition $f_{O3,s}(d)$ depends on the damage caused by O₃ during the current AND the previous hours $f_{O3,s}(h)$ and $f_{O3,s}(h-1)$ respectively (eq.5);
- there is a dose threshold under which there is no damage ($P_{\gamma1}/P_{\gamma2}$ in eq.6);
- the recovery from O₃ damage depends on leaf age according to the f_{LA} function (young leaves resist higher O₃ concentrations and can recover completely from O₃ damage within a period ranging from hours to a few days, Saxe 1991);

$$\begin{aligned} f_{O3,s}(d) &= f_{O3,s}(h) \cdot f_{O3,s}(h-1) & \text{for } h = 2, 3 \dots 24 \\ f_{O3,s}(d) &= f_{O3,s}(h) \cdot r_{O3,s} & \text{for } h = 1 \end{aligned} \quad (5)$$

With:

$$f_{O3,s}(h) = \begin{cases} 1 & \text{if } O_{3,up} \leq P_{\gamma1}/P_{\gamma2} \\ 1 + P_{\gamma1} - P_{\gamma2} \cdot O_{3,up} & \text{if } P_{\gamma1}/P_{\gamma2} < O_{3,up} < \frac{1+P_{\gamma1}}{P_{\gamma2}} \\ 0 & \text{if } O_{3,up} \geq \frac{1+P_{\gamma1}}{P_{\gamma2}} \end{cases} \quad (6)$$

And:

$$r_{O3,s} = f_{O3,s}(d-1) + [f_{O3,s}(h-1)] \cdot f_{LA} \quad (7)$$

Where $r_{O3,s}$ corresponds to the incomplete recovery from O₃ damage of the previous day (considering that repair of ozone damage during the night was not sufficient);

And where f_{LA} is a factor accounting for leaf age, with values between 0 and 1; f_{LA} equals to 1 before emergence, decreases linearly with the age of the leaf (°C.day) and falls to zero when the leaf is dead. Thus before emergence $r_{O3,s} = 1$ and for mature leaves there is quite no repair during the night ($r_{O3,s} \approx f_{O3,s}(d-1)$) (figure 1).

Finally this short-term photosynthesis inhibition factor $f_{O3,s}(d)$ reduces the Rubisco-limited rate of photosynthesis A_c (simulated at hourly steps as in the biochemical model of photosynthesis developed by Farquhar et al., 1980 and von Caemmerer & Farquhar, 1981):

$$A_{c,O3} = A_c \cdot f_{O3,s}(d) \cdot f_{LS} \quad (8)$$

The f_{LS} term in eq.8 is a senescence factor taking into account the natural decrease of the Rubisco-limited rate of photosynthesis with leaf senescence. As O₃ is assumed to accelerate senescence, this f_{LS} term is detailed below.

iii. O₃ effect on senescence

O₃ is assumed to accelerate the rate of senescence by reducing leaf life-span $t_{l,ma}$ through a long-term O₃ impact factor $f_{O3,l}$ calculated as a function of accumulated ozone uptake (till the leaf age t_l):

$$\begin{aligned} f_{O3,l} &= 1 - P_{\gamma3} \int_0^{t_l} O_{3,up} dt \\ t_{l,ma} &= (t_{l,ep} + t_{l,se}) \cdot f_{O3,l} \end{aligned} \quad (10)$$

Where $t_{l,ma}$ is the life-span of a mature leaf, corresponding to the thermal time from sowing to fully expanded leaf stage ($t_{l,ep}$) plus the thermal time during which the leaf is senescing $t_{l,se}$. O_3 is thus also assumed to bring forward the onset of senescence ($t_{l,se}=0.33t_{l,ma}$, Porter, 1984).

Finally, the factor f_{LS} accounting for the effect of senescence on the Rubisco-limited rate of photosynthesis A_c , is calculated taking into account the effect of accumulated ozone uptake (eq.11)

$$f_{LS} = \begin{cases} 1 & \text{before the fully expanded leaf stage} \\ 1 - \frac{a_l - t_{l,ep}}{t_{l,ma}/f_{O3,l} - t_{l,ep}} & \text{for } t_{l,em} < a_l < t_l \\ 0 & \text{for } a_l \geq t_l \end{cases} \quad (11)$$

Where a_l is the leaf age ($^{\circ}\text{Cday}$) and t_l is the leaf life-span ($^{\circ}\text{Cday}$)

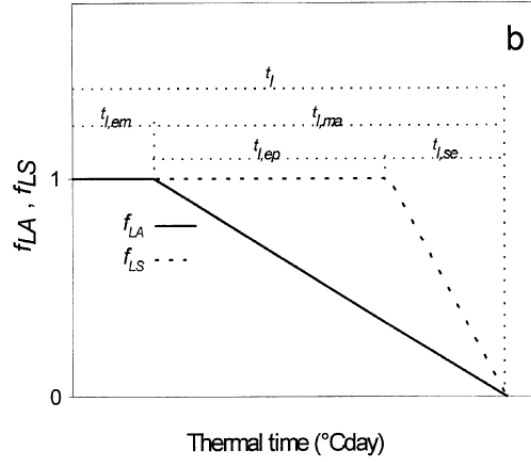


Figure 1: f_{LA} and f_{LS} factors versus the thermal time (from Ewert & Porter, 2000)

c. Van Oijen et al., 2004

i. O_3 inflow

The **daily damaging O_3 uptake** $QO_{3,up}$ is calculated according to the canopy stomatal conductance for CO_2 and O_3 g_s , the photoperiod average of ambient ozone concentration $[O_{3,aph}]$, and taking into account that part of the flux that is detoxified by inert plant material (cell walls) and by biochemical detoxification mechanisms $P_{f_{detox}}$:

$$QO_{3,up} = [O_{3,aph}] \cdot g_s \cdot (1 - P_{f_{detox}}) \quad (12)$$

ii. O_3 effect on photosynthesis

The daily radiation use efficiency $RUE(d)$ is reduced by a factor $F_{O3}(d)$ accounting for the daily photoperiod average of ambient ozone concentration $[O_{3,aph}]$ (and not for the daily damaging O_3 uptake previously calculated $QO_{3,up}$ eq.12 !):

$$RUE_{O3}(d) = RUE(d) \cdot F_{O3}(d) \quad (13)$$

With:

$$F_{O3}(d) = 1 - \frac{44}{30} \frac{[O_{3,aph}] \cdot P_{f_{detox}} \cdot P_{c_{detox}}}{C_a - C_i} - f_{lv} \cdot P_{f_{repair}} \quad (14)$$

Where the ratio $44/30$ is the ratio of carbon contents of CO_2 ($12/44$) and CH_2O ($12/30$), f_{lv} is the fraction of produced assimilates that is allocated to leaf growth and maintenance, f_{repair} is the fraction of assimilates allocated to leaves that is used in

repair, P_{Cdetox} is the cost coefficient of detoxification, C_a is ambient CO_2 concentration, C_i is the leaf internal CO_2 concentration (supposed to be equal to $0.7 C_a$).

iii. O_3 effect on senescence

Nothing is proposed by the authors to deal with the O_3 impact on senescence.

d. *Lebard with CERES-O3, 2005*

i. O_3 inflow

The **damaging instantaneous O_3 uptake rate within the leaf layer II** $O_{3,up,ll}$ is calculated according to the stomatal conductance for O_3 , g_{O3} , the ambient ozone concentration near leaf surface in the leaf layer II, $[O_{3,a,ll}]$, and taking into account that a part of the flux is detoxified accordingly to the leaf age:

$$O_{3,up,ll} = ([O_{3,a,ll}] - P_{Kd} \cdot Facsen) \cdot g_{O3} \cdot 10^{-12} \quad (15)$$

Where $Kd \cdot g_{O3} \cdot Facsen$ corresponds to the instantaneous detoxified flux in layer II, and $Kd \cdot Facsen$ is a threshold concentration above which O_3 impacts the crop growth. This threshold evolves according to the leaf senescence which is estimated through to ratio between the actual leaf photosynthesis activity and the maximal (before senescence) leaf photosynthesis activity:

$$Facsen = \frac{V_{cmax}}{P_{V_{cmaxopt}}} \quad (16)$$

A **damaging cumulative amount of O_3** is then calculated (t in second):

$$CO_{3,up,ll} = \int_0^t O_{3,up,ll} \cdot 3600 \cdot dt \quad (17)$$

ii. O_3 effect on photosynthesis

The maximum rate of carboxylation V_{cmax} is reduced according to the damaging cumulative amount of O_3 , $CO_{3,up,ll}$ (eq.17):

$$V_{cmax,O3} = V_{cmax} - P_{Ki} \cdot 10^{-3} \cdot CO_{3,up,ll} \quad (18)$$

Where P_{Ki} is an O_3 impact coefficient.

The Rubisco amount is also reduced by the damaging instantaneous O_3 uptake rate within the leaf layer II $O_{3,up,ll}$ calculated as described above (eq.15)

$$\partial RU = -P_{Ki} \cdot [RU] \cdot O_{3,up,ll} + \partial RU_{remobilisation} \quad (19)$$

Where δRU is the variation of the stock of Rubisco, P_{Ki} is an impact coefficient ($= 302 s^{-1}$), $[RU]$ is the remaining amount of Rubisco, and $\delta RU_{remobilisation}$ is the reduction of the stock of Rubisco because of remobilization.

This formalism allows simulating the cumulative effect of O_3 as well as the dose effect on the photosynthesis response to the cumulative effect (Fig.2).

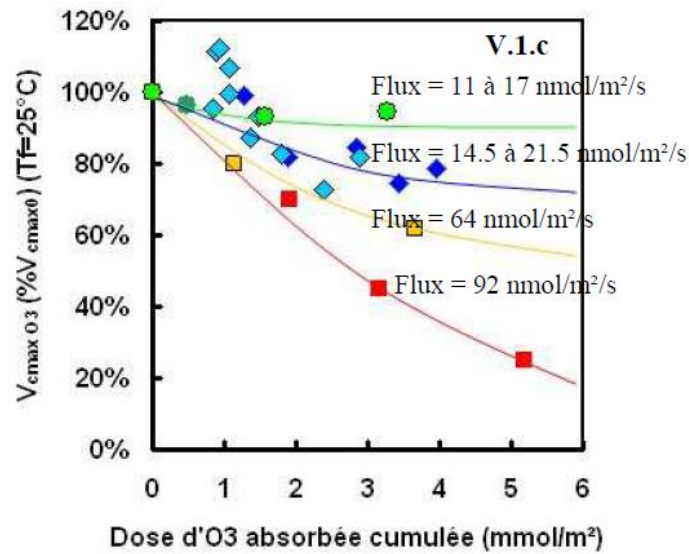


Figure 2: Maximum carboxylation rate versus cumulative O₃ uptake and according to the average O₃ inflow (from Lebard, 2005, Fig. V.1.c Chap. V.)

iii. O₃ effect on senescence

Nothing is proposed by the author to deal with the O₃ impact on senescence.

Furthermore, the author developed a formalism about the O₃ impact on leaf nitrogen content.

e. Synthesis on about threshold effect, detoxification and repair mechanisms, and time scales which are considered in the previous modelling approaches.

Model	O3 Influx			O3 impacts					
	time step and secondary effects	comment	equation	time step and secondary effects	comment	equation	time step and secondary effects	comment	equation
Kobayashi (Kobayashi, 1997)	daily threshold effect	The O ₃ influx is not calculated, but a damaging [O ₃] is calculated. the threshold [O ₃] air is supposed to be constant	eq. 1	daily leaf age effect on the repair capacity	2 sensitivity parameters are fixed, one for the vegetative growth, and one for the reproductive growth	eq. 2 eq. 2	daily	daily senescent rate is increased by daily damaging O ₃ uptake	eq. 3
AFRCWHEAT2-O3 (Ewert & Porter, 2000)	instantaneous (second)		eq. 4	hourly threshold effect leaf age effect on the repair capacity	O ₃ effect on the Rubisco-limited rate of photosynthesis Ac (FvCB model) low O ₃ concentration are detoxified without direct effect on the photosynthetic system; but the reduced detoxification capacity with leaf age is not taken into account (Pell et al., 1997) young leaves can recover fully from O ₃ damage (Pell et al., 1992)	eq. 5 eq. 6 eq. 7	daily?	cumulative effect of O ₃ on senescence	eq. 10
van Oijen (van Oijen et al., 2004)	daily threshold effect	the O ₃ flux that is instantaneously detoxified is cut away in order to directly calculate a damaging O ₃ uptake	eq. 12	daily threshold effect no leaf age effect	O ₃ effect on the RUE the cost of O ₃ detoxification is taken into account the cost of leaf repair is taken into account as a constant parameter	eq. 13 eq. 14 eq. 14			
CERES-O3 (Lebard, 2005)	instantaneous (second) threshold effect leaf age effect on instantaneous detoxification (Pell et al., 1997)	The damaging instantaneous O ₃ uptake rate is calculated for every leaf layers	eq. 15	hourly	damaging O ₃ cumulative amount effect on the maximum rate of carboxylation Vcmax (FvCB model)	eq. 18			

2. Conceptual framework of the future STICS O₃ module

In order to build an O₃ module pluggable to STICS, it's necessary to choose formalisms using input variables that can be provided by STICS (or at less calculated from STICS state variables). As STICS assesses daily canopy resistances for CO₂ exchanges through a resistive approach (Fig. 3), and simulates a daily net photosynthesis according to an integrative approach without downscaling to the biochemical processes such as in the FvCB model, we propose the following formalisms in line with van Oijen et al. (2004) and Lebart (2005).

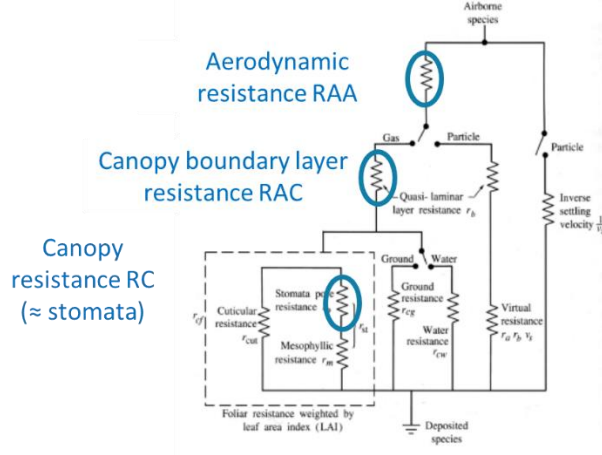


Figure 3: Canopy resistances as calculated by STICS (from Brisson et al., 2009)

a. O₃ inflow

In line with van Oijen et al. (2004), the **daily damaging O₃ uptake** $QO_{3,up}$ (nmol.m⁻² ground.day⁻¹) is calculated according to the canopy resistance for O₃ (the inverse of canopy conductance for O₃), the photoperiod average of ambient ozone concentration $[O_{3,aph}]$ (nmol.m⁻² ground.s⁻¹), and taking into account that part of the flux that is instantaneously detoxified $P_{f_{detox}}$ (eq. 20). The canopy resistance for O₃ is the canopy resistance for CO₂ RT (sm⁻¹) corrected for the differences in the diffusivities of CO₂ and O₃ in the air with the ratio P_{kdifO_3} (eq. 20). Two options were implemented, considering only the stomatal resistance rc (1st option) which is the greater contribution, or alternatively all resistances (2nd option) i.e. aerodynamic resistance raa , canopy boundary layer resistance rac and stomatal resistance rc (eq. 21):

$$QO_{3,up}(d) = 1/RT(d) \cdot [O_{3,aph}] \cdot P_{kdifO_3} \cdot (1 - P_{f_{detox}}) \cdot photoperiod \cdot 3600 \quad (20)$$

$$\text{Where} \quad RT(d) = \begin{cases} rc(d) & \text{if option 1} \\ rc(d) + rac(d) + raa(d) & \text{if option 2} \end{cases} \quad (21)$$

The **damaging cumulative amount of O₃** $CO_{3,up}$ (mmol O₃ m⁻²ground) is thus equal to:

$$CO_{3,up}(d) = \int_{em}^d QO_{3,up}(i) \cdot 10^{-6} \quad (22)$$

b. O₃ impact on photosynthesis

In line with Lebard (2005), we consider the cumulative effect of O₃ on photosynthesis, as well as the dose effect on the photosynthesis response to the cumulative effect. We apply Lebard approach (eq.18, fig.2) to the maximum value of the radiation use efficiency $EBMAX$ (eq. 23, Fig. 4):

$$\frac{EBMAX_{O_3}(d)}{EBMAX(d)} = 1 - \left(1 - \exp(-f_{FO_3} \cdot CO_{3,up}(d))\right) \quad (23)$$

With : $f_{FO_3} = P_kdose_{O_3} \cdot FO_{3,up}(d)$ (24)

Where: $FO_{3,up} = QO_{3,up} / (\text{photoperiod} \cdot 3600)$ (25)

EBMAXO₃ is the maximum radiation use efficiency under O₃ effect (g biomass.MJ⁻¹) while EBMAX is the maximum radiation use efficiency without O₃ effect. CO_{3,up} as calculated in eq.22, represents the cumulative amount of O₃ uptake, whereas f_{FO₃} is the O₃ dose effect factor on photosynthesis response to the cumulative effect of O₃. f_{FO₃} is calculated from FO_{3,up} (eq.24) i.e. the instantaneous average of O₃ inflow calculated from the daily damaging O₃ uptake QO_{3,up} (eq.25). P_kdose_{O₃} is a coefficient supposed to be constant.

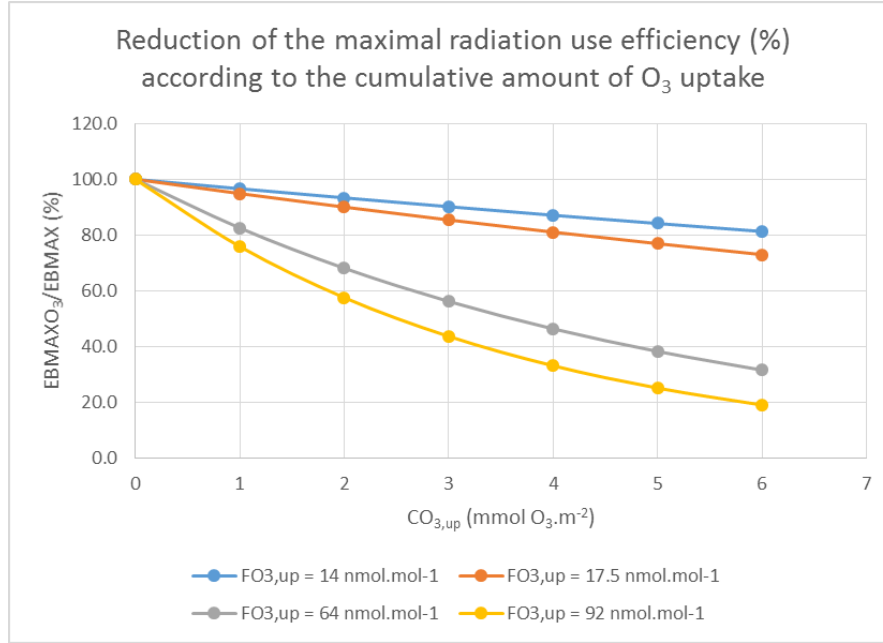


Figure 4: Relation between the reduction of the maximum radiation use efficiency and the cumulative amount of O₃ uptake, according to the inflow intensity

3. Parameterization, evaluation and perspectives of the STICS O₃ module

Parameters of the O₃ module should now be estimated:

- The ratio of diffusion rates **P_kdifO₃** is fixed at 0.93 when considering only the stomatal resistance (1st option), according to Ewert and Porter (2000). When considering all resistances (2nd option) i.e. aerodynamic resistance r_{aa}, canopy boundary layer resistance r_{ac} and stomatal resistance r_c, we should estimate a diffusion ratio for each of them: the diffusion ratio for aerodynamic resistance could be fixed at 1 (A. Olioso, com. Pers.), and the diffusion ratio for boundary layer resistance should be found in the literature.
- The instantaneous detoxified fraction of O₃ flux **P_f_{detox}** is fixed at 0.9 according to van Oijen et al. (2004).
- The coefficient for the O₃ dose effect factor calculation **P_kdose_{O₃}** is estimated from the V_{cmaxO₃}/V_{cmax} curve by Lebard (2005) originally established with data from Lebard (2005), Farage et al. (1991) and Cardoso Vilhena et al. (2004) (see Lebard, 2005, Figure V.1). The optimized value of P_kdose_{O₃} is thus fixed at 3.10⁻³.

The O₃ module should be evaluated, and parameters estimated more accurately, according to data found in the literature (such as Farage et al., 1991, Ewert et al., 1999; Cardoso Vilhena et al., 2004 and Lebard, 2005) and from the ozone experiments conducted by Danish colleagues in Roskilde University and DTU within the Climate CAFÉ project (Hansen et al., 2019).

Finally, the effect of leaf age on the detoxification efficiency could be introduced into the module, by transforming the $P_{f_{\text{detox}}}$ parameter into a variable evolving with leaf age. Last, the effect of O₃ on senescence has to be formalized.

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Annex 1: Table of Parameters, Input and Output variables in models from Kobayashi (1997), Ewert and Porter (2000), van Oijen et al. (2004) and Lebard (2005).

Name	Input variable / Output variable / Parameter	Definition	Unit	Value (for parameters only)	Equation	Model / Reference	Time step calculation
[O ₃](d)	Output variable	Daily mean O ₃ concentration in excess of background O ₃ (day d)	ppb or nmol.mol ⁻¹	not estimated by author	1	Kobayashi, 1997	daily average
[O _{3,a}](d)	Input variable	Daily mean O ₃ concentration in the air (day d)	ppb or nmol.mol ⁻¹		1	Kobayashi, 1997	daily average
P_[O _{3,b}]	Parameter	Background O ₃ concentration (under which there is no damage)	ppb or nmol.mol ⁻¹		1	Kobayashi, 1997	
RUE(d)	Input variable	Daily radiation use efficiency with no O ₃ impact	g biomass.MJ ⁻¹	not estimated by author	2	Kobayashi, 1997	daily
RUEO ₃ (d)	Output variable	Daily radiation use efficiency reduced by O ₃ impact	g biomass.MJ ⁻¹		2	Kobayashi, 1997	daily
P_pveg	Parameter	sensitivity of photosynthesis to excess O ₃ during vegetative growth	-		2	Kobayashi, 1997	
P_prep	Parameter	sensitivity of photosynthesis and senescence to excess O ₃ during reproductive growth	-	not estimated by author	2	Kobayashi, 1997	
LAI(d)	Output variable	Daily LAI	m ² leaves . m ⁻² soil	not estimated by author	3	Kobayashi, 1997	daily
LAI _{max}	Input variable	maximum LAI	m ² leaves . m ⁻² soil		3	Kobayashi, 1997	crop season maximum
P_α _r	Parameter	constant rate of LAI decrease from the end of vegetative growth (<=> senescence)	-		3	Kobayashi, 1997	
O _{3,up}	Output variable	Instantaneous O ₃ uptake rate (flux)	nmol.m ⁻² .s ⁻¹	0.93	4	Ewert&Porter, 2000	instantaneous (second)
[O _{3,a}]	Input variable	Instantaneous O ₃ concentration at the leaf surface	ppb or nmol.mol ⁻¹		4	Ewert&Porter, 2000	hourly average
g _{sc}	Input variable	Stomatal conductance for CO ₂	mol.m ⁻² .s ⁻¹		4	Ewert&Porter, 2000	hourly
P_fO ₃	Parameter	ratio of diffusion rates for O ₃ and CO ₂	-	0.93	4	Ewert&Porter, 2000	
f _{O_{3,s}} (d)	Output variable	short-term O ₃ dose effect factor [0,1] inhibiting photosynthesis and accounting for the damage caused during the current and previous hours	-	0.06	5	Ewert&Porter, 2000	hourly
f _{O_{3,s}} (h)	Output variable	short-term O ₃ dose effect factor [0,1] accounting for the damage caused during the current hour	-		5	Ewert&Porter, 2000	hourly
P_γ ₁	Parameter	O ₃ short-term damage coefficient	-		6	Ewert&Porter, 2000	
P_γ ₂	Parameter	O ₃ short-term damage coefficient	(nmol.m ⁻² .s ⁻¹) ⁻¹	0.0045	6	Ewert&Porter, 2000	
P_γ ₃	Parameter	O ₃ long-term damage coefficient	(nmol.m ⁻² .s ⁻¹) ⁻¹	0.5	10	Ewert&Porter, 2000	
A _{c,O₃}	Output variable	Rubisco-limited rate of carboxylation (during photosynthesis) reduced by O ₃ effect	μmol.m ⁻² .s ⁻¹	0.9	8	Ewert&Porter, 2000	instantaneous (second)
A _c	Output variable	Rubisco-limited rate of carboxylation (during photosynthesis)	μmol.m ⁻² .s ⁻¹		8	Ewert&Porter, 2000	instantaneous (second)
f _{LA}	Output variable	factor accounting for leaf age [0,1]	-		7	Ewert&Porter, 2000	daily
f _{LS}	Output variable	factor accounting for leaf senescence [0,1]	-	0.05	8, 11	Ewert&Porter, 2000	daily
t _{l,ma}	Output variable	life-span of a mature leaf	°C.day		10, 11	Ewert&Porter, 2000	daily
t _{l,ep}	Input variable	thermal time from sowing to fully expanded leaf stage	°C.day		10, 11	Ewert&Porter, 2000	daily
t _{l,em}	Input variable	thermal time from sowing to emergence	°C.day	0.05	10, 11	Ewert&Porter, 2000	daily
t _{l,se}	Input variable	thermal time during which the leaf is senescing	°C.day		10	Ewert&Porter, 2000	daily
f _{O_{3,l}}	Output variable	long-term O ₃ impact factor [0,1] accelerating senescence	-		10	Ewert&Porter, 2000	daily
t _l	Output variable	life-span of the leaf	°C.day	0.05	10	Ewert&Porter, 2000	daily
a _l	Output variable	leaf age	°C.day		11	Ewert&Porter, 2000	daily
P_fdetox	Parameter	detoxified fraction of O ₃ flux	-	0.9	12	van Oijen et al., 2004	daily
QO _{3,up}	Output variable	Daily damaging O ₃ uptake rate (flux)	g O ₃ .m ⁻² ground.day ⁻¹	0.375	12	van Oijen et al., 2004	daily
g _s	Input variable	Stomatal conductance for CO ₂ and O ₃ (supposed to be equal)	mol.m ⁻² .s ⁻¹		12	van Oijen et al., 2004	instantaneous (second)
[O _{3,a,ph}]	Input variable	photoperiod average of ambient ozone concentration	ml O ₃ .m ⁻³		12	van Oijen et al., 2004	daily average
RUE(d)	Input variable	Daily radiation use efficiency with no O ₃ impact	g biomass.MJ ⁻¹	0.05	13	van Oijen et al., 2004	daily
RUEO ₃ (d)	Output variable	Daily radiation use efficiency reduced by O ₃ impact	g biomass.MJ ⁻¹		13	van Oijen et al., 2004	daily
F _{O₃} (d)	Output variable	O ₃ effect factor [0,1] inhibiting photosynthesis	-		13	van Oijen et al., 2004	daily
P_cdetox	Parameter	cost coefficient of detoxification	g CH ₂ O g ⁻¹ detoxified	0.375	14	van Oijen et al., 2004	
f _{lv}	Input variable	fraction of assimilates allocated to leaf growth and maintenance	g.g ⁻¹	0.05	14	van Oijen et al., 2004	daily
P_frepair	Parameter	fraction of assimilates allocated to leaves that is used in repair	g.g ⁻¹		14	van Oijen et al., 2004	
Ca	Input variable	ambient CO ₂ concentration	ml CO ₂ m ⁻³		14	van Oijen et al., 2004	daily
Ci	Input variable	leaf internal CO ₂ concentration	ml CO ₂ m ⁻³		14	van Oijen et al., 2004	daily
O _{3,up,II}	Output variable	Damaging instantaneous O ₃ uptake rate within the leaf layer II (flux)	nmol.m ⁻² .s ⁻¹	49.4	15	Lebard, 2005	instantaneous (second)
[O _{3,a,II}]	Input variable	Instantaneous O ₃ concentration at the leaf surface in leaf layer II	ppb or nmol.mol ⁻¹		15	Lebard, 2005	hourly average
P_Kd	Parameter	Coefficient of instantaneous detoxification and repair	ppb or nmol.mol ⁻¹		15	Lebard, 2005	
Facsen	Output variable	Factor of senescence effect on the threshold of damaging instantaneous O ₃ uptake	-	95	15	Lebard, 2005	instantaneous (second)
V _{Cmax,O₃}	Output variable	Maximum rate of carboxylation reduced by absorbed O ₃	μmol.m ⁻² leaf.s ⁻¹		18	Lebard, 2005	instantaneous (second)
V _{Cmax}	Output variable	Maximum rate of carboxylation	μmol.m ⁻² leaf.s ⁻¹		16	Lebard, 2005	instantaneous (second)
P_V _{Cmaxopt}	Parameter	Maximum rate of carboxylation for an optimum nitrogen content in leaves	μmol.m ⁻² leaf.s ⁻¹	95	16	Lebard, 2005	instantaneous (second)
CO _{3,up,II}	Output variable	Damaging cumulative amount of uptaken O ₃	mmol.m ⁻² leaf	302	17	Lebard, 2005	over the crop season
P_Ki	Parameter	Coefficient of O ₃ impact	s ⁻¹		18	Lebard, 2005	

Annex 2: Table of Parameters, Input and Output variables of the STICS O3 module

Name	Input variable / Output variable / Parameter	Definition	Unit	Value (for parameters only)	Equation	Comment
QO _{3,up}	Output variable	Daily damaging O ₃ uptake	nmol O ₃ .m ⁻² ground.day ⁻¹		20	
RT	Input variable	Canopy resistance for CO ₂	(mol.m ⁻² .s ⁻¹) ⁻¹		20, 21	
[O _{3,ap}]	Input variable	photoperiod average of ambient ozone concentration	nmol.mol ⁻¹ or ppb		20	
P _{_kdifO₃}	Parameter	ratio of diffusion rates for O ₃ and CO ₂	-	0.93	20	From Ewert & Porter (2000)
P _{_f_{detox}}	Parameter	detoxified fraction of O ₃ flux	-	0.9	20	From van Oijen et al. (2004)
photoperiod	Input variable	Daily interval period during which the plants are exposed to light	hour		20, 25	
RT	Input variable	Canopy resistance for CO ₂	(mol.m ⁻² .s ⁻¹) ⁻¹		21	
rc	Input variable	Stomatal resistance for CO ₂	(mol.m ⁻² .s ⁻¹) ⁻¹		21	
raa	Input variable	Aerodynamic resistance for CO ₂	(mol.m ⁻² .s ⁻¹) ⁻¹		21	
rac	Input variable	Boundary layer resistance for CO ₂	(mol.m ⁻² .s ⁻¹) ⁻¹		21	
CO _{3,up}	Output variable	Damaging cumulative amount of O ₃ uptake	mmol O ₃ .m ⁻² ground		22	
EBMAX _{O₃}	Output variable	Maximum radiation use efficiency under O ₃ effect	g biomass.MJ ⁻¹		23	
EBMAX	Input variable	Maximum radiation use efficiency without O ₃	g biomass.MJ ⁻¹		23	
fFO ₃	Output variable	O ₃ dose effect factor on photosynthesis response to the cumulative effect of O ₃	(mmol O ₃ .m ⁻² ground) ⁻¹		23, 24	
P _{_kdoseO₃}	Parameter	coefficient for the O ₃ dose effect factor calculation	10 ⁻⁶ .(nmol O ₃) ⁻¹ .m ⁴ ground.day	0.003	24	estimated from Lebard (2005) with data from Lebard (2005) and Farage et al. (1991) and Cardoso Vilhena et al. (2004)
FO _{3,up}	Output variable	Instantaneous damaging O ₃ uptake rate (flux)	nmol O ₃ .m ⁻² ground.s ⁻¹		25	